



# wwPDB X-ray Structure Validation Summary Report

Mar 12, 2026 – 05:49 PM UTC


PDB ID : 4KHP / pdb\_00004khp  
Title : Structure of the Thermus thermophilus 30S ribosomal subunit in complex with de-6-MSA-pactamycin  
Authors : Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2013-05-01  
Resolution : 3.10 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

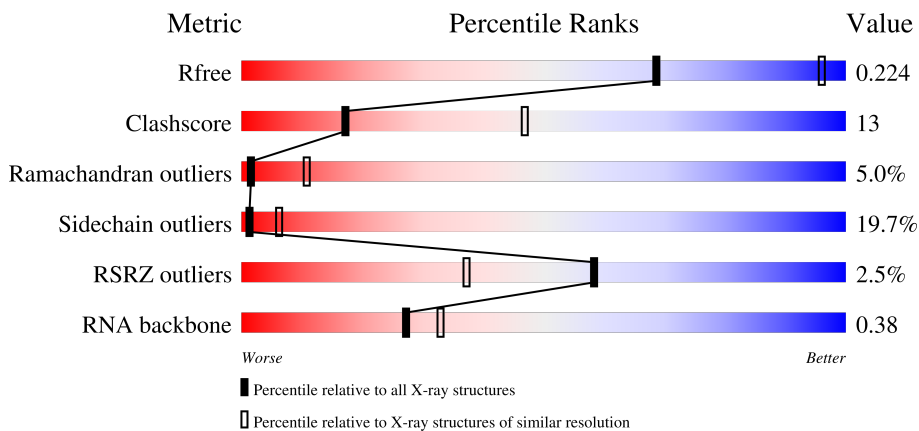
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



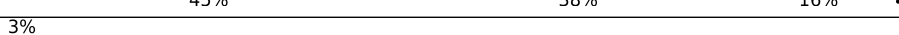
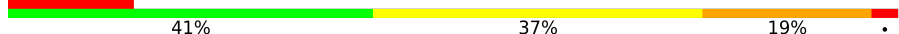
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1506	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">45%      36%      15%      .</p>
2	B	234	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">6%      48%      38%      13%      .</p>
3	C	206	<div style="display: flex; align-items: center;"> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">60%      33%      .      .</p>
4	D	208	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">5%      62%      27%      7%      .</p>

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Mol	Chain	Length	Quality of chain
5	E	150	 64% 24% 10% .
6	F	101	 58% 35% 7%
7	G	155	 66% 29% 5%
8	H	138	 63% 28% 8% .
9	I	127	 48% 35% 16% .
10	J	98	 38% 46% 15% .
11	K	119	 66% 29% 6%
12	L	125	 61% 25% 13% .
13	M	120	 45% 38% 16% .
14	N	60	 47% 32% 13% 8%
15	O	88	 67% 24% 8% .
16	P	83	 60% 34% 6%
17	Q	99	 69% 25% 6%
18	R	70	 66% 30% . .
19	S	78	 41% 37% 19% .
20	T	99	 56% 33% 7% .
21	U	24	 58% 42%
22	X	6	 33% 17% 17% 33%

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 52032 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1506	32368	14408	5997	10458	1505	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	A	G	conflict	GB 55771382

- Molecule 2 is a protein called 30S Ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S Ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	155	1257	781	252	218	6	0	0	0

- Molecule 8 is a protein called 30S Ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	138	1116	705	215	193	3	0	0	0

- Molecule 9 is a protein called 30S Ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1011	639	198	174	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	794	499	156	138	1	0	0	0

- Molecule 11 is a protein called 30S Ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S Ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	975	614	196	164	1	0	0	0

- Molecule 13 is a protein called 30S Ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	120	955	591	197	165	2	0	0	0

- Molecule 14 is a protein called 30S Ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S Ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S Ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called 30S Ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 30S Ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	70	574	367	112	95	0	0	0

- Molecule 19 is a protein called 30S Ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	78	Total 629	C 403	N 114	O 110	S 2	0	0	0

- Molecule 20 is a protein called 30S Ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	Total 763	C 470	N 162	O 129	S 2	0	0	0

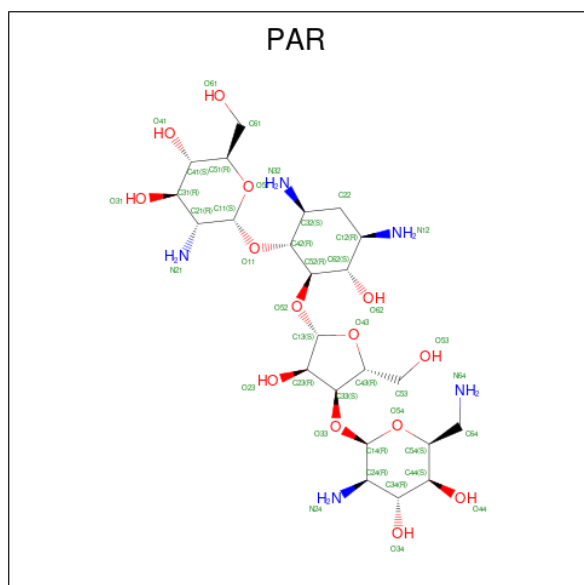
- Molecule 21 is a protein called 30S Ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	U	24	Total 208	C 128	N 50	O 30	0	0	0

- Molecule 22 is a RNA chain called Fragment of messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	X	6	Total 117	C 54	N 14	O 44	P 5	0	0	0

- Molecule 23 is PAROMOMYCIN (CCD ID: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



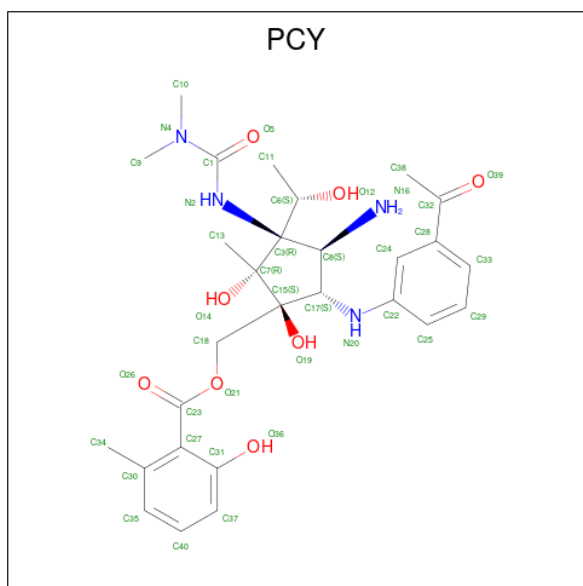
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	A	1	Total 42	C 23	N 5	O 14	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	A	1	Total	C	N	O	0	0
			42	23	5	14		
23	A	1	Total	C	N	O	0	0
			42	23	5	14		
23	A	1	Total	C	N	O	0	0
			42	23	5	14		
23	A	1	Total	C	N	O	0	0
			42	23	5	14		
23	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 24 is Pactamycin (CCD ID: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	Total	C	N	O	0	0
			30	20	4	6		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	A	99	Total	Mg	0	0
			99	99		
25	D	1	Total	Mg	0	0
			1	1		

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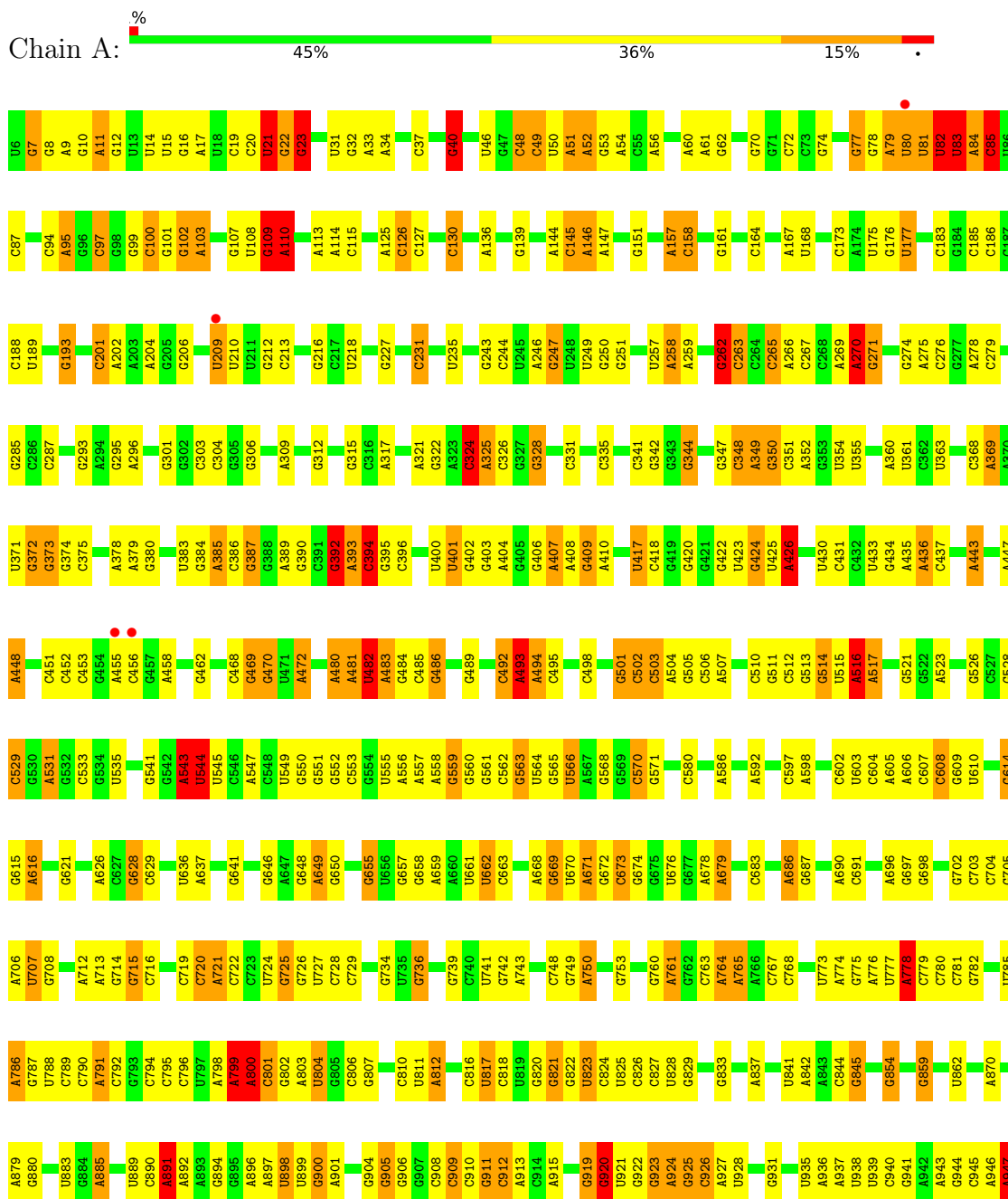
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
25	E	1	Total 1	Mg 1	0	0
25	K	1	Total 1	Mg 1	0	0
25	S	1	Total 1	Mg 1	0	0

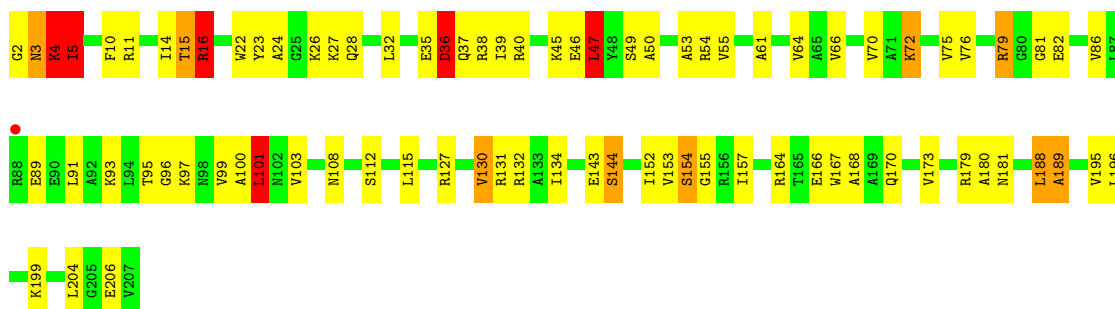
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

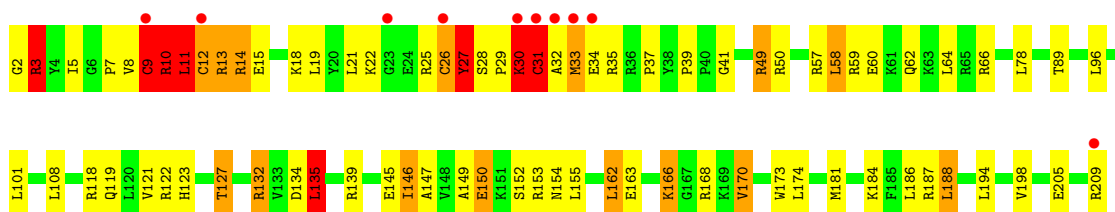
- Molecule 1: 16S Ribosomal RNA



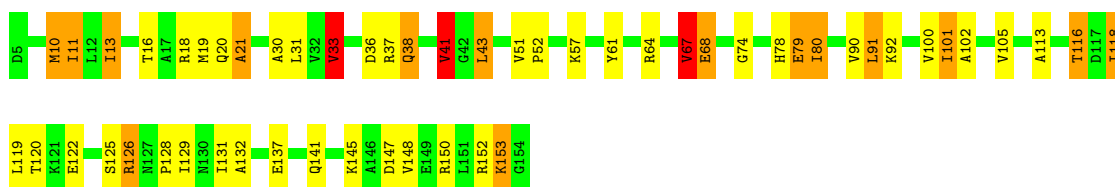




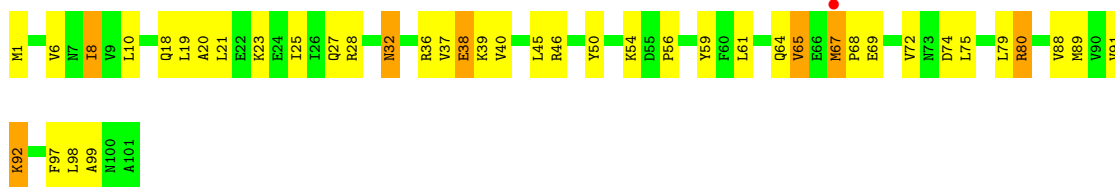
- Molecule 4: 30S Ribosomal protein S4



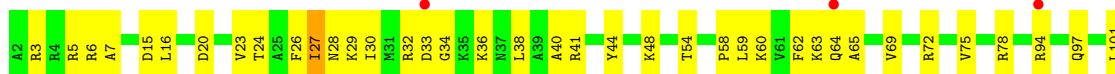
- Molecule 5: 30S Ribosomal protein S5



- Molecule 6: 30S Ribosomal protein S6



- Molecule 7: 30S Ribosomal protein S7

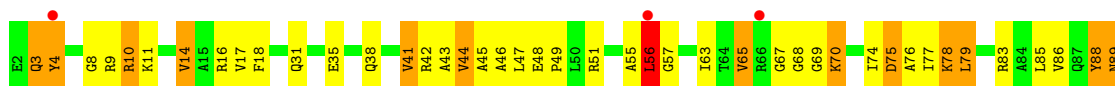




- Molecule 8: 30S Ribosomal protein S8



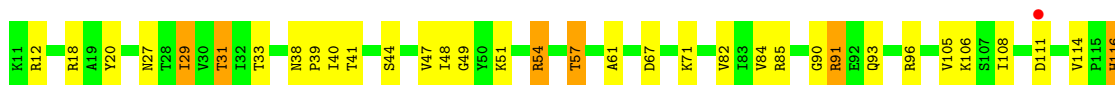
- Molecule 9: 30S Ribosomal protein S9



- Molecule 10: 30S Ribosomal protein S10

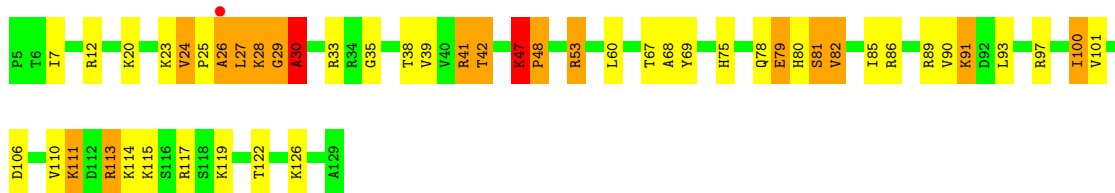


- Molecule 11: 30S Ribosomal protein S11

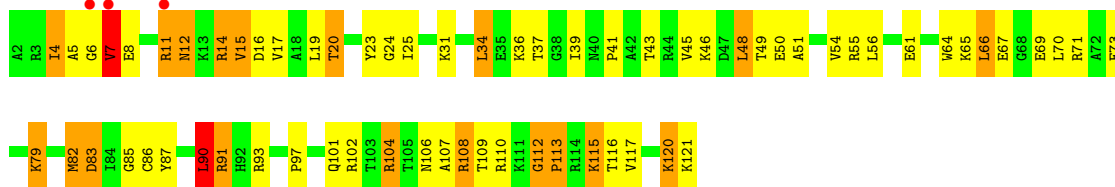
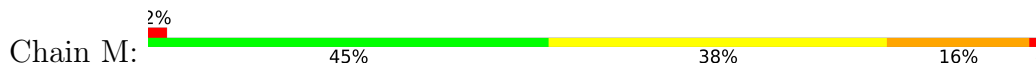


- Molecule 12: 30S Ribosomal protein S12

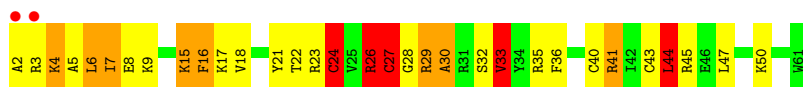




- Molecule 13: 30S Ribosomal protein S13



- Molecule 14: 30S Ribosomal protein S14



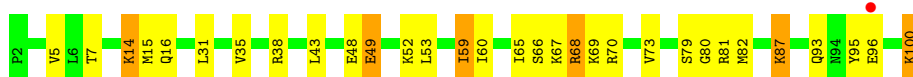
- Molecule 15: 30S Ribosomal protein S15



- Molecule 16: 30S Ribosomal protein S16



- Molecule 17: 30S Ribosomal protein S17

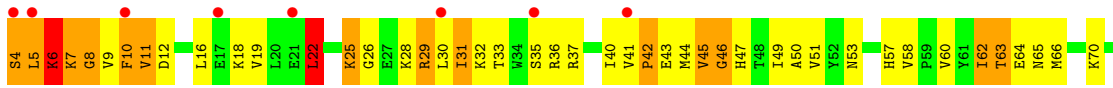


- Molecule 18: 30S Ribosomal protein S18

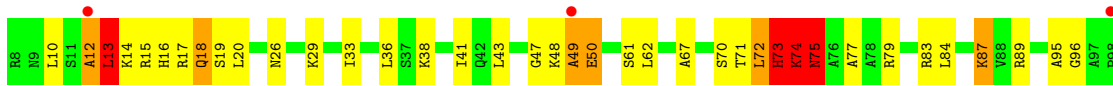




- Molecule 19: 30S Ribosomal protein S19



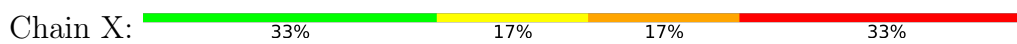
- Molecule 20: 30S Ribosomal protein S20



- Molecule 21: 30S Ribosomal protein THX



- Molecule 22: Fragment of messenger RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.00Å 401.00Å 176.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 3.10 29.67 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.67-3.10) 91.3 (29.67-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 3.11Å)	Xtrriage
Refinement program	REFMAC 5.8.0031	Depositor
R, $R_{free}$	0.185 , 0.226 0.188 , 0.224	Depositor DCC
$R_{free}$ test set	11726 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	52032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, PCY, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	4/36233 (0.0%)	1.10	338/56552 (0.6%)
2	B	0.84	0/1935	1.11	0/2609
3	C	0.90	1/1636 (0.1%)	1.07	3/2205 (0.1%)
4	D	0.92	2/1733 (0.1%)	1.20	13/2318 (0.6%)
5	E	0.98	2/1162 (0.2%)	1.19	5/1564 (0.3%)
6	F	0.73	0/856	1.00	2/1154 (0.2%)
7	G	0.73	0/1276	1.03	4/1709 (0.2%)
8	H	0.94	0/1136	1.24	6/1527 (0.4%)
9	I	0.74	1/1029 (0.1%)	1.06	1/1378 (0.1%)
10	J	0.82	0/807	1.12	2/1085 (0.2%)
11	K	0.82	0/900	1.08	0/1213
12	L	0.98	0/991	1.21	4/1327 (0.3%)
13	M	0.80	0/965	1.12	3/1292 (0.2%)
14	N	1.04	0/501	1.32	7/664 (1.1%)
15	O	0.82	0/745	1.04	1/992 (0.1%)
16	P	0.87	0/716	1.09	1/963 (0.1%)
17	Q	0.88	0/836	1.07	2/1117 (0.2%)
18	R	0.72	0/579	0.98	0/768
19	S	0.79	0/642	1.02	2/865 (0.2%)
20	T	0.93	2/765 (0.3%)	1.20	2/1007 (0.2%)
21	U	0.78	0/212	1.04	0/277
22	X	0.60	0/128	1.14	2/196 (1.0%)
All	All	0.67	12/55783 (0.0%)	1.10	398/82782 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
11	K	0	1
12	L	0	2
14	N	0	1
19	S	0	1
20	T	0	3
All	All	0	11

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CA-CB	8.33	1.67	1.53
1	A	82	U	O3'-P	7.80	1.72	1.61
1	A	83	U	O3'-P	6.97	1.71	1.61
3	C	4	LYS	N-CA	6.79	1.54	1.46
20	T	13	LEU	CA-C	6.42	1.61	1.52

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	C	C2'-C3'-O3'	15.97	133.46	109.50
1	A	1050	A	C2'-C3'-O3'	14.11	130.66	109.50
1	A	469	G	C2'-C3'-O3'	13.16	129.24	109.50
1	A	82	U	C2'-C3'-O3'	12.86	128.78	109.50
1	A	1047	G	C2'-C3'-O3'	-12.48	90.78	109.50

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	LYS	Peptide
4	D	31	CYS	Peptide
8	H	109	ILE	Peptide
11	K	116	HIS	Peptide
12	L	26	ALA	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32368	0	16339	537	0
2	B	1900	0	1951	86	0
3	C	1612	0	1677	43	0
4	D	1703	0	1763	63	0
5	E	1146	0	1207	45	0
6	F	843	0	857	23	0
7	G	1257	0	1296	28	0
8	H	1116	0	1177	29	0
9	I	1011	0	1043	50	0
10	J	794	0	840	46	0
11	K	885	0	904	22	0
12	L	975	0	1062	38	0
13	M	955	0	1021	38	0
14	N	492	0	529	31	0
15	O	734	0	771	14	0
16	P	700	0	720	26	0
17	Q	823	0	891	18	0
18	R	574	0	644	16	0
19	S	629	0	652	38	0
20	T	763	0	861	29	0
21	U	208	0	221	4	0
22	X	117	0	64	2	0
23	A	294	0	315	26	0
24	A	30	0	31	5	0
25	A	99	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	K	1	0	0	0	0
25	S	1	0	0	0	0
All	All	52032	0	36836	1116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:C:H2'	1:A:1232:A:C8	1.70	1.18
1:A:1287:G:N2	1:A:1313:G:O2'	1.80	1.13
5:E:101:ILE:HD11	5:E:119:LEU:HD23	1.31	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:27:CYS:O	14:N:27:CYS:SG	2.20	0.98
1:A:1232:A:O2'	1:A:1233:A:H8	1.46	0.97

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	180 (78%)	39 (17%)	13 (6%)	1	8
3	C	204/206 (99%)	156 (76%)	33 (16%)	15 (7%)	1	5
4	D	206/208 (99%)	172 (84%)	23 (11%)	11 (5%)	1	10
5	E	148/150 (99%)	127 (86%)	20 (14%)	1 (1%)	18	49
6	F	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	6	25
7	G	153/155 (99%)	128 (84%)	22 (14%)	3 (2%)	6	25
8	H	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	18	49
9	I	125/127 (98%)	99 (79%)	15 (12%)	11 (9%)	0	3
10	J	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	10
11	K	117/119 (98%)	102 (87%)	8 (7%)	7 (6%)	1	7
12	L	123/125 (98%)	98 (80%)	16 (13%)	9 (7%)	1	5
13	M	118/120 (98%)	88 (75%)	17 (14%)	13 (11%)	0	2
14	N	58/60 (97%)	40 (69%)	12 (21%)	6 (10%)	0	2
15	O	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	3	16
16	P	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	5	25
18	R	68/70 (97%)	60 (88%)	7 (10%)	1 (2%)	8	32
19	S	76/78 (97%)	55 (72%)	15 (20%)	6 (8%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/99 (98%)	81 (84%)	7 (7%)	9 (9%)	0	3
21	U	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2342/2382 (98%)	1924 (82%)	300 (13%)	118 (5%)	1	11

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	18	GLY
2	B	44	LEU
2	B	226	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/202 (100%)	155 (77%)	47 (23%)	1	4
3	C	160/160 (100%)	126 (79%)	34 (21%)	1	5
4	D	180/180 (100%)	149 (83%)	31 (17%)	2	10
5	E	115/115 (100%)	94 (82%)	21 (18%)	2	8
6	F	90/90 (100%)	74 (82%)	16 (18%)	2	9
7	G	126/126 (100%)	107 (85%)	19 (15%)	3	13
8	H	119/119 (100%)	96 (81%)	23 (19%)	1	7
9	I	98/98 (100%)	74 (76%)	24 (24%)	1	3
10	J	88/88 (100%)	67 (76%)	21 (24%)	1	3
11	K	90/90 (100%)	74 (82%)	16 (18%)	2	9
12	L	104/104 (100%)	86 (83%)	18 (17%)	2	9
13	M	96/96 (100%)	73 (76%)	23 (24%)	1	3
14	N	49/49 (100%)	34 (69%)	15 (31%)	0	0
15	O	79/79 (100%)	66 (84%)	13 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	72/72 (100%)	62 (86%)	10 (14%)	3	15
17	Q	94/94 (100%)	82 (87%)	12 (13%)	4	18
18	R	61/61 (100%)	51 (84%)	10 (16%)	2	11
19	S	69/69 (100%)	50 (72%)	19 (28%)	0	1
20	T	76/76 (100%)	61 (80%)	15 (20%)	1	6
21	U	19/19 (100%)	14 (74%)	5 (26%)	0	2
All	All	1987/1987 (100%)	1595 (80%)	392 (20%)	1	6

5 of 392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	87	THR
13	M	101	GLN
11	K	31	THR
12	L	67	THR
14	N	24	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN
11	K	78	GLN
20	T	75	ASN
9	I	124	GLN
10	J	78	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1506 (99%)	348 (23%)	66 (4%)
22	X	5/6 (83%)	3 (60%)	0
All	All	1510/1512 (99%)	351 (23%)	66 (4%)

5 of 351 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	10	G

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Mol	Chain	Res	Type
1	A	21	U
1	A	23	G
1	A	32	G

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1234	A
1	A	1301	A
1	A	1507	G
1	A	516	A
1	A	514	G

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 103 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	PAR	A	1604	-	44,45,45	0.88	2 (4%)	63,67,67	1.90	13 (20%)
23	PAR	A	1601	-	44,45,45	0.79	1 (2%)	63,67,67	2.03	15 (23%)
23	PAR	A	1605	-	44,45,45	0.80	0	63,67,67	2.14	17 (26%)
23	PAR	A	1603	-	44,45,45	0.76	2 (4%)	63,67,67	1.97	11 (17%)
23	PAR	A	1607	-	44,45,45	1.15	4 (9%)	63,67,67	2.12	21 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PCY	A	1608	-	23,31,42	1.38	2 (8%)	25,49,65	1.56	4 (16%)
23	PAR	A	1602	-	44,45,45	0.81	1 (2%)	63,67,67	1.72	15 (23%)
23	PAR	A	1606	-	44,45,45	0.74	0	63,67,67	2.01	17 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PAR	A	1604	-	-	9/18/94/94	0/4/4/4
23	PAR	A	1601	-	-	2/18/94/94	0/4/4/4
23	PAR	A	1605	-	-	12/18/94/94	0/4/4/4
23	PAR	A	1603	-	-	6/18/94/94	0/4/4/4
23	PAR	A	1607	-	-	8/18/94/94	1/4/4/4
24	PCY	A	1608	-	-	2/26/60/67	0/2/2/3
23	PAR	A	1602	-	-	7/18/94/94	0/4/4/4
23	PAR	A	1606	-	-	11/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1608	PCY	C28-C32	-4.01	1.42	1.49
23	A	1607	PAR	C31-C21	-3.94	1.48	1.53
24	A	1608	PCY	C22-N20	-3.35	1.33	1.39
23	A	1604	PAR	C13-C23	-3.28	1.48	1.52
23	A	1607	PAR	C22-C32	-2.73	1.48	1.53

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1605	PAR	C14-O54-C54	7.29	127.95	113.72
23	A	1601	PAR	C44-C34-C24	6.63	121.99	110.99
23	A	1603	PAR	O33-C14-C24	5.86	117.66	108.08
23	A	1603	PAR	C14-O33-C33	-5.61	104.69	117.98
23	A	1603	PAR	O34-C34-C24	-5.52	100.31	110.22

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1602	PAR	C23-C13-O52-C52
23	A	1602	PAR	O43-C13-O52-C52
23	A	1603	PAR	C23-C13-O52-C52
23	A	1603	PAR	O43-C13-O52-C52
23	A	1603	PAR	C44-C54-C64-N64

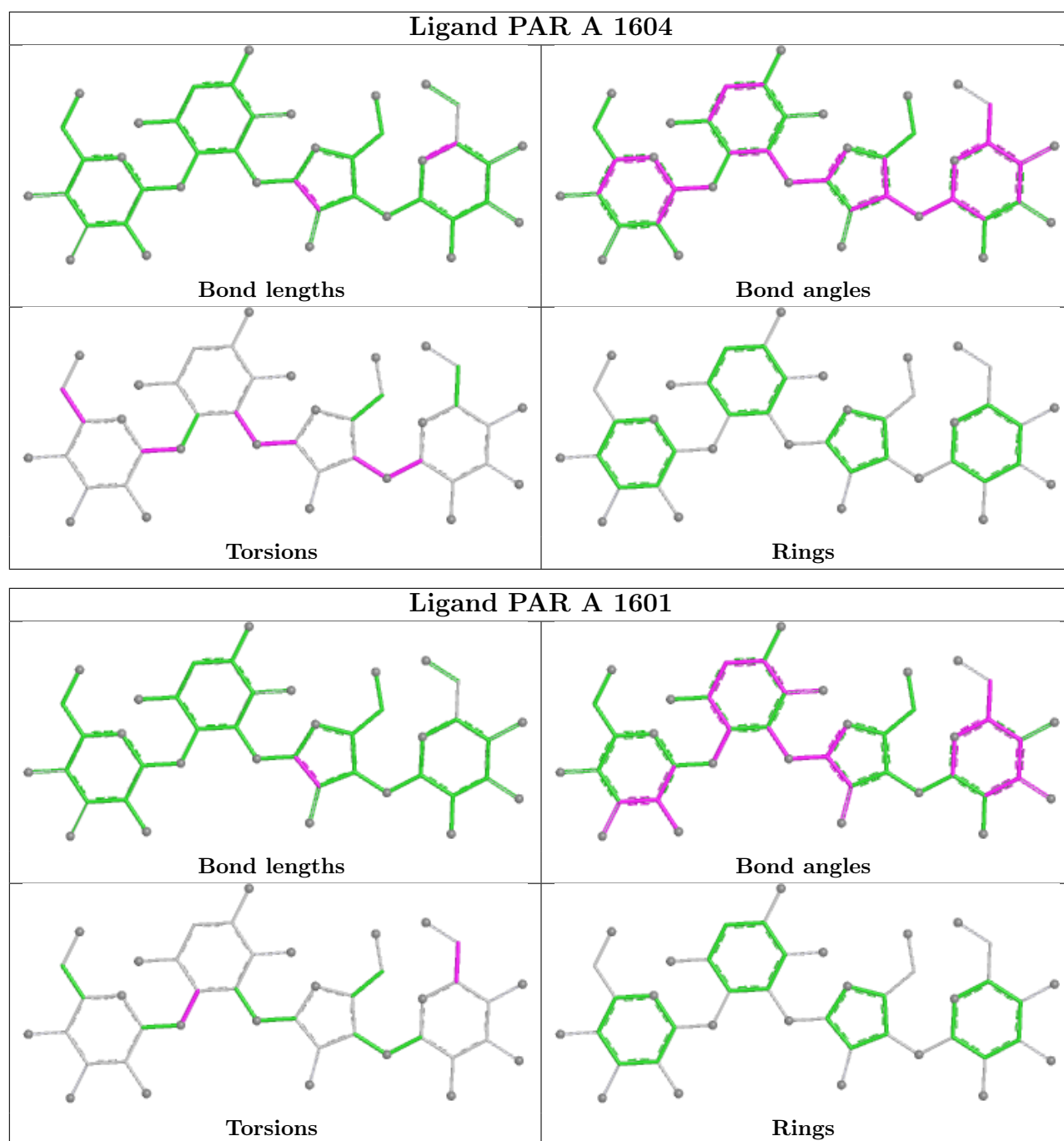
All (1) ring outliers are listed below:

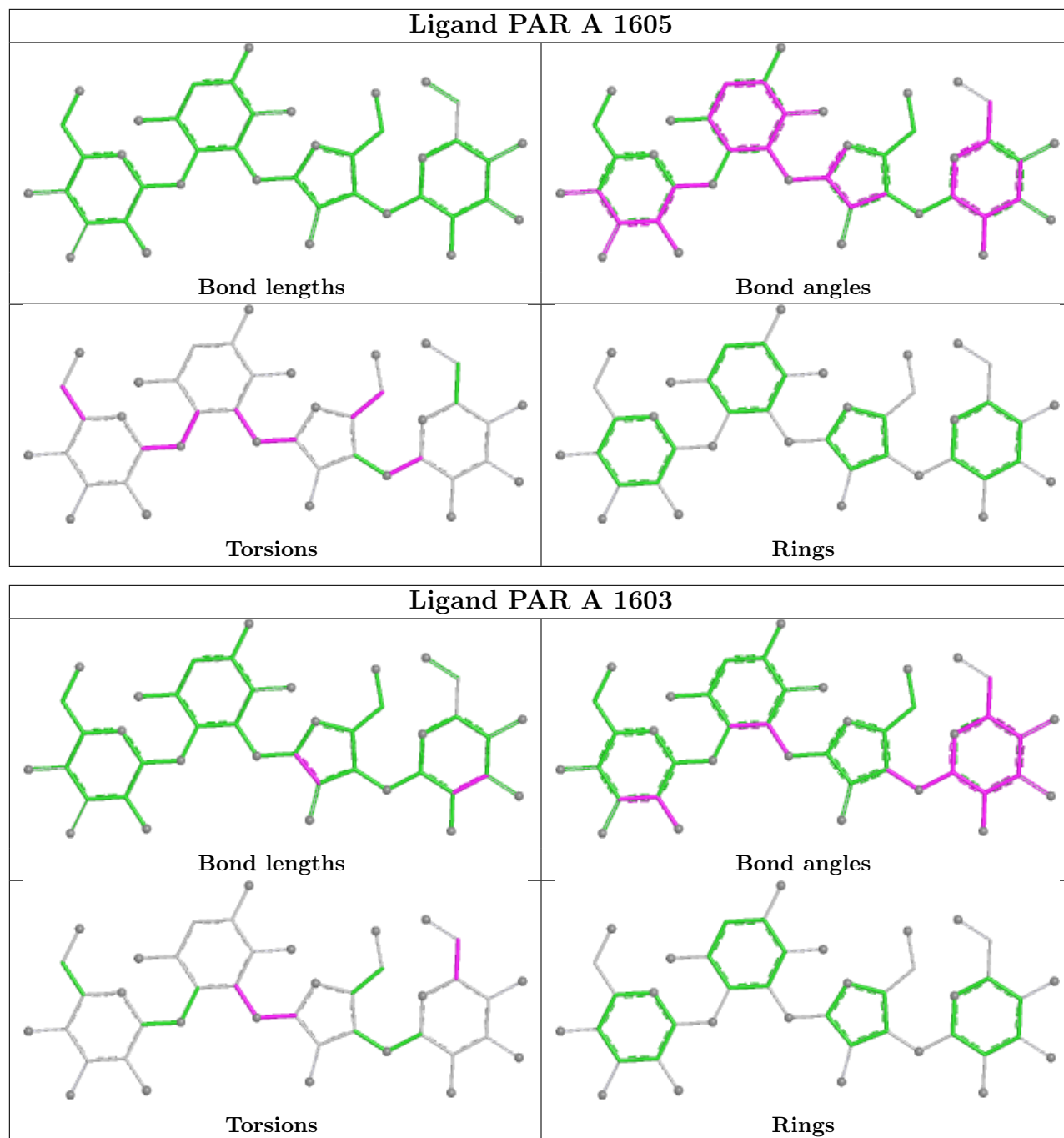
Mol	Chain	Res	Type	Atoms
23	A	1607	PAR	C12-C22-C32-C42-C52-C62

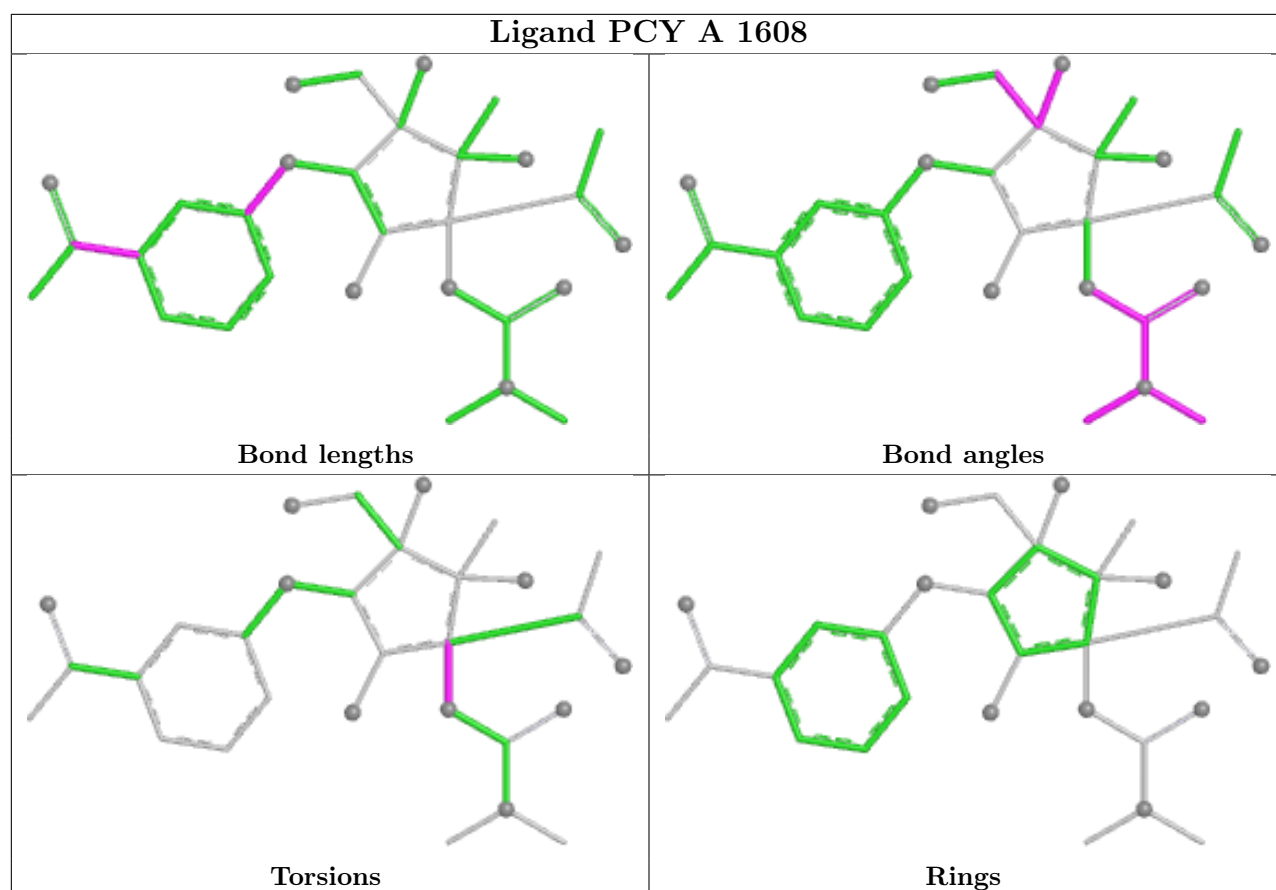
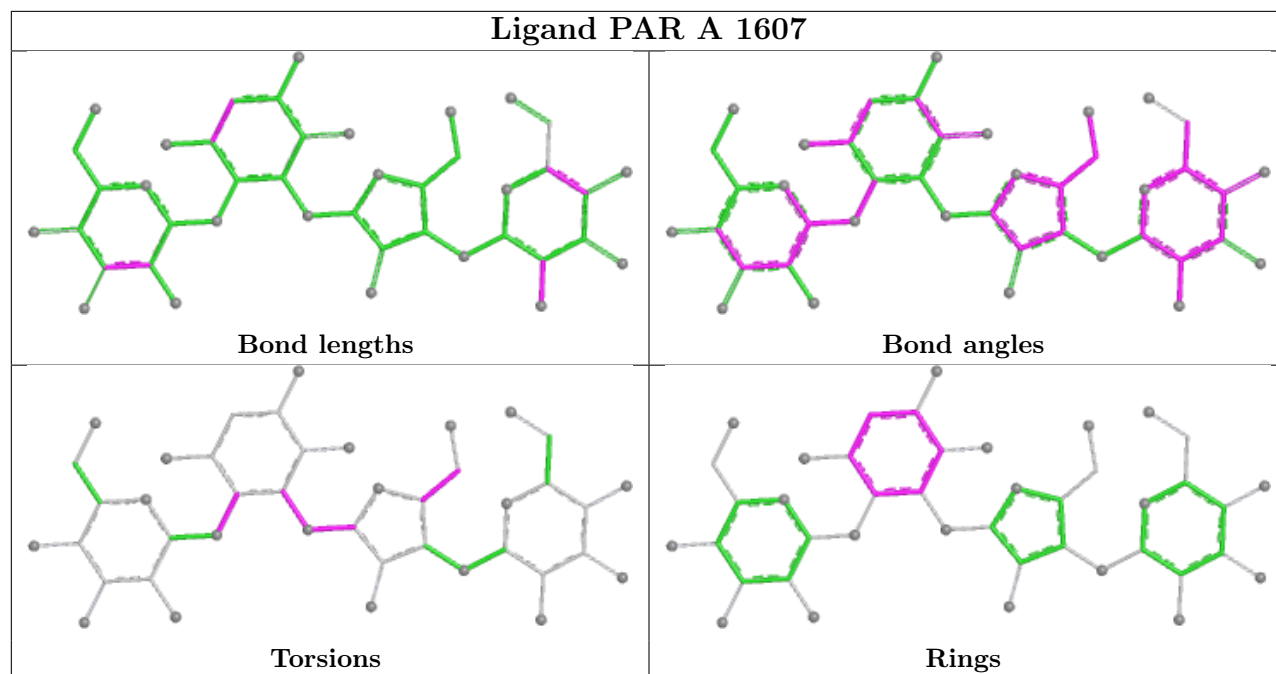
6 monomers are involved in 31 short contacts:

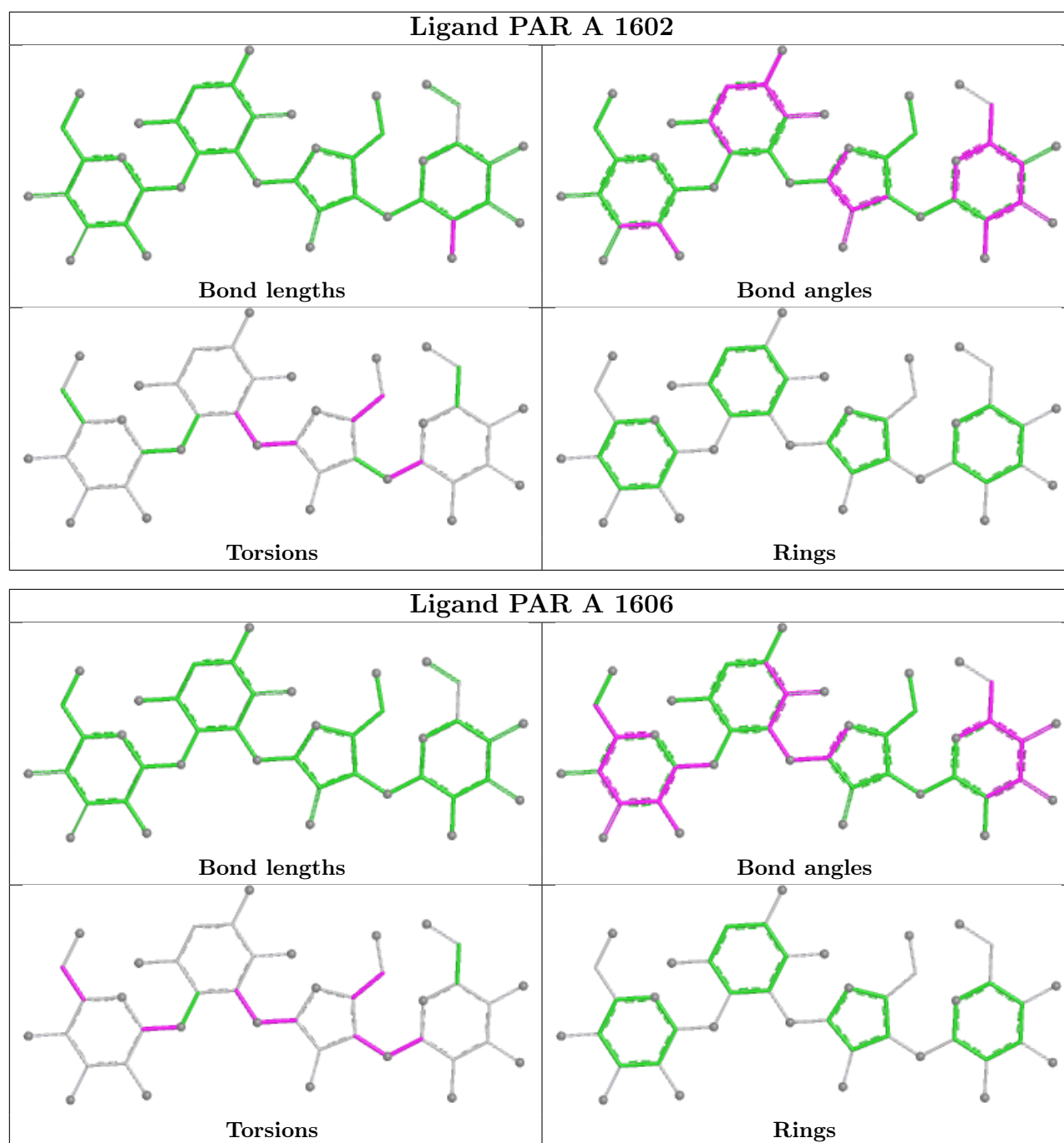
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1604	PAR	8	0
23	A	1601	PAR	3	0
23	A	1605	PAR	1	0
23	A	1603	PAR	6	0
23	A	1607	PAR	8	0
24	A	1608	PCY	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1506/1506 (100%)	-0.36	22 (1%) 72 52	39, 69, 142, 245	0
2	B	234/234 (100%)	0.39	15 (6%) 25 14	53, 98, 168, 194	0
3	C	206/206 (100%)	0.25	1 (0%) 87 73	55, 95, 139, 157	0
4	D	208/208 (100%)	0.11	10 (4%) 35 19	53, 80, 113, 134	0
5	E	150/150 (100%)	-0.23	0 100 100	41, 65, 98, 136	0
6	F	101/101 (100%)	0.10	1 (0%) 79 61	72, 101, 131, 172	0
7	G	155/155 (100%)	0.27	5 (3%) 50 30	65, 96, 145, 196	0
8	H	138/138 (100%)	-0.33	2 (1%) 73 53	40, 61, 91, 131	0
9	I	127/127 (100%)	0.46	4 (3%) 51 30	51, 103, 140, 219	0
10	J	98/98 (100%)	0.89	10 (10%) 12 6	61, 126, 174, 199	0
11	K	119/119 (100%)	0.04	4 (3%) 48 28	53, 78, 113, 164	0
12	L	125/125 (100%)	-0.02	1 (0%) 82 65	39, 76, 112, 179	0
13	M	120/120 (100%)	0.29	3 (2%) 58 37	60, 97, 144, 183	0
14	N	60/60 (100%)	0.27	2 (3%) 49 29	62, 85, 113, 131	0
15	O	88/88 (100%)	-0.10	1 (1%) 78 59	55, 82, 121, 155	0
16	P	83/83 (100%)	-0.23	0 100 100	50, 67, 99, 140	0
17	Q	99/99 (100%)	-0.20	1 (1%) 79 61	42, 72, 106, 142	0
18	R	70/70 (100%)	-0.05	1 (1%) 73 53	61, 81, 123, 157	0
19	S	78/78 (100%)	0.66	11 (14%) 6 3	72, 114, 168, 186	0
20	T	99/99 (100%)	0.22	4 (4%) 42 23	51, 78, 136, 162	0
21	U	24/24 (100%)	0.45	1 (4%) 40 22	67, 82, 111, 134	0
22	X	6/6 (100%)	0.23	0 100 100	59, 75, 131, 138	0
All	All	3894/3894 (100%)	-0.05	99 (2%) 58 37	39, 79, 145, 245	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	26	CYS	6.5
1	A	1017	G	5.1
9	I	4	TYR	4.9
1	A	1233	A	4.8
19	S	10	PHE	4.7

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
25	MG	A	1676	1/1	0.79	0.32	51,51,51,51	0
25	MG	A	1663	1/1	0.83	0.35	64,64,64,64	0
25	MG	A	1632	1/1	0.85	0.38	56,56,56,56	0
25	MG	A	1658	1/1	0.86	0.30	41,41,41,41	1
25	MG	D	301	1/1	0.86	0.20	93,93,93,93	0
25	MG	A	1613	1/1	0.88	0.27	56,56,56,56	1
25	MG	A	1639	1/1	0.88	0.32	47,47,47,47	0
25	MG	A	1707	1/1	0.89	0.41	67,67,67,67	0
25	MG	A	1697	1/1	0.89	0.34	63,63,63,63	0
25	MG	A	1700	1/1	0.90	0.09	52,52,52,52	0
25	MG	A	1691	1/1	0.90	0.63	69,69,69,69	0
25	MG	A	1673	1/1	0.90	0.25	41,41,41,41	1
25	MG	A	1680	1/1	0.91	0.31	36,36,36,36	1
25	MG	A	1684	1/1	0.91	0.24	67,67,67,67	1
25	MG	A	1690	1/1	0.91	0.20	54,54,54,54	0
25	MG	A	1626	1/1	0.91	0.27	31,31,31,31	0
25	MG	A	1671	1/1	0.91	0.41	57,57,57,57	1
25	MG	A	1636	1/1	0.91	0.20	46,46,46,46	0
25	MG	A	1675	1/1	0.91	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1662	1/1	0.91	0.28	48,48,48,48	0
25	MG	A	1683	1/1	0.92	0.23	44,44,44,44	1
25	MG	A	1670	1/1	0.92	0.39	49,49,49,49	1
25	MG	A	1647	1/1	0.92	0.24	34,34,34,34	0
25	MG	A	1651	1/1	0.92	0.37	42,42,42,42	0
23	PAR	A	1605	42/42	0.92	0.18	58,75,85,89	42
25	MG	A	1634	1/1	0.92	0.19	44,44,44,44	0
25	MG	A	1706	1/1	0.92	0.59	71,71,71,71	0
25	MG	A	1643	1/1	0.92	0.34	59,59,59,59	0
25	MG	A	1681	1/1	0.92	0.20	36,36,36,36	0
25	MG	A	1609	1/1	0.93	0.21	45,45,45,45	0
25	MG	A	1648	1/1	0.93	0.29	43,43,43,43	0
25	MG	A	1696	1/1	0.93	0.23	54,54,54,54	0
25	MG	A	1679	1/1	0.93	0.19	61,61,61,61	0
25	MG	A	1667	1/1	0.93	0.21	39,39,39,39	0
25	MG	A	1705	1/1	0.93	0.29	61,61,61,61	0
23	PAR	A	1603	42/42	0.93	0.16	53,84,97,117	42
25	MG	A	1622	1/1	0.93	0.27	38,38,38,38	0
25	MG	A	1659	1/1	0.93	0.48	36,36,36,36	1
25	MG	S	101	1/1	0.93	0.14	58,58,58,58	0
25	MG	A	1692	1/1	0.94	0.49	65,65,65,65	0
25	MG	A	1694	1/1	0.94	0.30	61,61,61,61	0
25	MG	A	1611	1/1	0.94	0.12	37,37,37,37	0
25	MG	A	1623	1/1	0.94	0.17	57,57,57,57	0
25	MG	A	1649	1/1	0.94	0.14	53,53,53,53	1
25	MG	A	1624	1/1	0.94	0.17	38,38,38,38	0
25	MG	A	1637	1/1	0.94	0.18	59,59,59,59	0
25	MG	A	1685	1/1	0.94	0.15	46,46,46,46	0
23	PAR	A	1607	42/42	0.94	0.20	11,15,17,19	42
25	MG	A	1627	1/1	0.94	0.28	50,50,50,50	0
25	MG	A	1635	1/1	0.95	0.18	42,42,42,42	0
23	PAR	A	1606	42/42	0.95	0.15	38,44,55,56	42
25	MG	A	1661	1/1	0.95	0.38	60,60,60,60	0
25	MG	A	1688	1/1	0.95	0.29	49,49,49,49	0
25	MG	A	1689	1/1	0.95	0.42	52,52,52,52	0
23	PAR	A	1604	42/42	0.95	0.13	64,79,104,137	0
25	MG	A	1638	1/1	0.95	0.28	40,40,40,40	0
25	MG	A	1666	1/1	0.95	0.18	47,47,47,47	0
25	MG	A	1620	1/1	0.95	0.23	34,34,34,34	0
25	MG	A	1628	1/1	0.95	0.31	39,39,39,39	0
25	MG	A	1645	1/1	0.95	0.14	34,34,34,34	0
25	MG	A	1630	1/1	0.95	0.38	33,33,33,33	1

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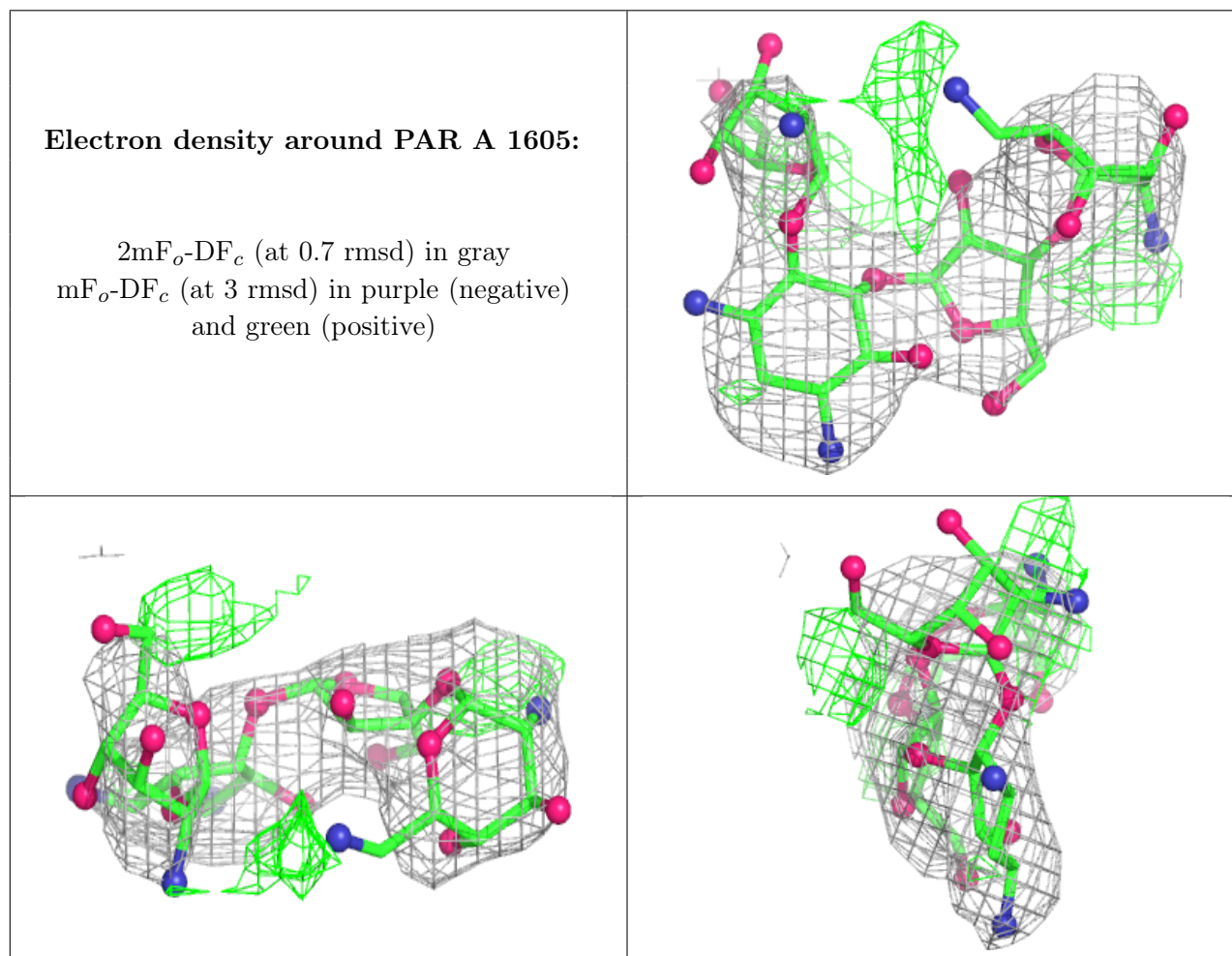
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1703	1/1	0.95	0.23	88,88,88,88	0
25	MG	A	1631	1/1	0.95	0.12	36,36,36,36	0
24	PCY	A	1608	30/40	0.95	0.10	50,59,68,76	0
25	MG	A	1650	1/1	0.95	0.13	37,37,37,37	0
23	PAR	A	1601	42/42	0.95	0.09	52,59,74,83	0
25	MG	A	1655	1/1	0.95	0.15	39,39,39,39	1
25	MG	A	1652	1/1	0.96	0.21	49,49,49,49	0
25	MG	A	1695	1/1	0.96	0.28	64,64,64,64	0
25	MG	A	1619	1/1	0.96	0.16	25,25,25,25	0
25	MG	A	1664	1/1	0.96	0.24	61,61,61,61	0
25	MG	A	1686	1/1	0.96	0.32	42,42,42,42	1
25	MG	A	1701	1/1	0.96	0.47	68,68,68,68	0
25	MG	A	1702	1/1	0.96	0.15	51,51,51,51	0
25	MG	A	1625	1/1	0.96	0.24	50,50,50,50	0
25	MG	A	1633	1/1	0.96	0.38	52,52,52,52	0
25	MG	A	1669	1/1	0.96	0.26	57,57,57,57	0
23	PAR	A	1602	42/42	0.96	0.10	32,41,50,61	42
25	MG	A	1682	1/1	0.96	0.14	52,52,52,52	0
25	MG	A	1693	1/1	0.96	0.25	52,52,52,52	0
25	MG	A	1617	1/1	0.97	0.21	35,35,35,35	0
25	MG	A	1641	1/1	0.97	0.09	42,42,42,42	0
25	MG	A	1677	1/1	0.97	0.26	58,58,58,58	0
25	MG	A	1678	1/1	0.97	0.07	54,54,54,54	0
25	MG	A	1614	1/1	0.97	0.17	31,31,31,31	0
25	MG	A	1665	1/1	0.97	0.05	40,40,40,40	0
25	MG	A	1644	1/1	0.97	0.14	41,41,41,41	0
25	MG	A	1698	1/1	0.97	0.17	53,53,53,53	0
25	MG	A	1699	1/1	0.97	0.23	55,55,55,55	0
25	MG	A	1615	1/1	0.97	0.24	38,38,38,38	0
25	MG	A	1668	1/1	0.97	0.21	39,39,39,39	1
25	MG	A	1646	1/1	0.97	0.19	34,34,34,34	0
25	MG	A	1621	1/1	0.97	0.19	45,45,45,45	0
25	MG	A	1704	1/1	0.97	0.13	53,53,53,53	0
25	MG	A	1660	1/1	0.97	0.41	61,61,61,61	0
25	MG	A	1687	1/1	0.97	0.19	43,43,43,43	1
25	MG	A	1672	1/1	0.97	0.33	65,65,65,65	0
25	MG	A	1616	1/1	0.97	0.38	40,40,40,40	0
25	MG	K	201	1/1	0.97	0.50	52,52,52,52	0
25	MG	A	1674	1/1	0.97	0.06	49,49,49,49	0
25	MG	A	1654	1/1	0.98	0.11	26,26,26,26	0
25	MG	A	1640	1/1	0.98	0.18	36,36,36,36	0
25	MG	A	1656	1/1	0.98	0.20	50,50,50,50	0

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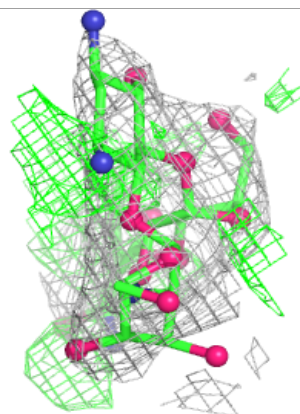
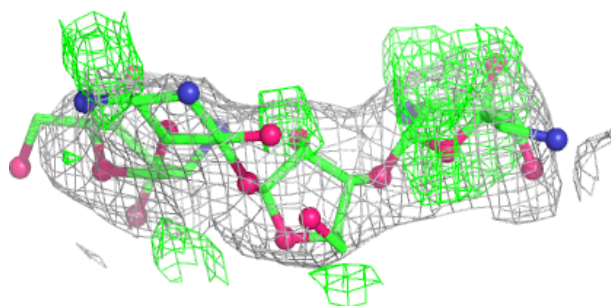
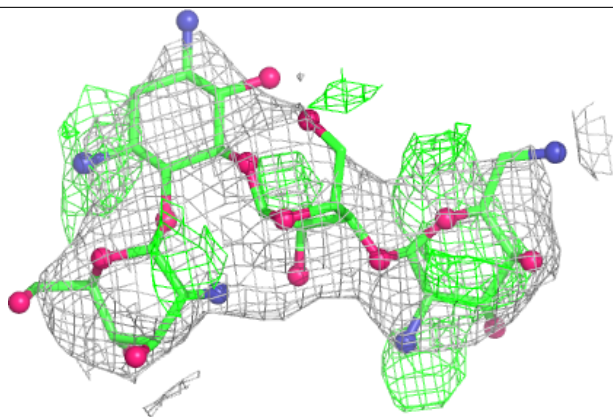
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	A	1610	1/1	0.98	0.24	42,42,42,42	0
25	MG	A	1629	1/1	0.98	0.17	42,42,42,42	0
25	MG	E	201	1/1	0.98	0.21	39,39,39,39	0
25	MG	A	1612	1/1	0.98	0.31	46,46,46,46	0
25	MG	A	1653	1/1	0.98	0.21	30,30,30,30	0
25	MG	A	1618	1/1	0.99	0.43	56,56,56,56	0
25	MG	A	1642	1/1	0.99	0.32	43,43,43,43	0
25	MG	A	1657	1/1	0.99	0.07	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

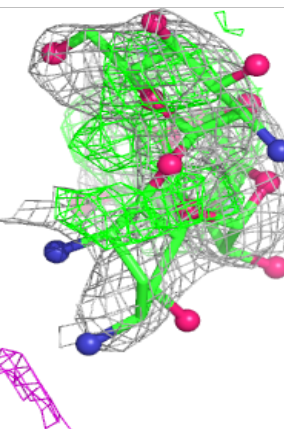
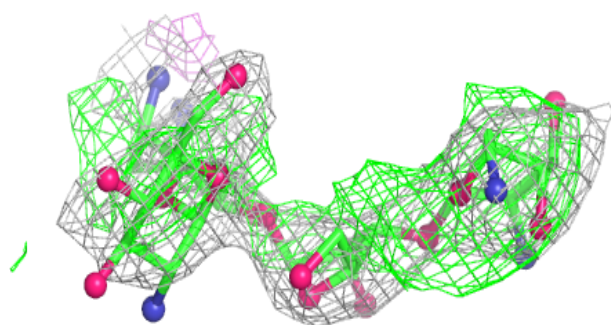
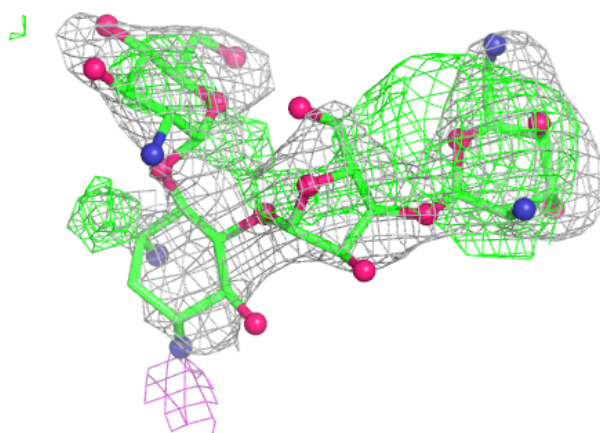


**Electron density around PAR A 1603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

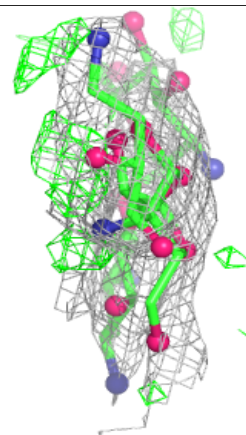
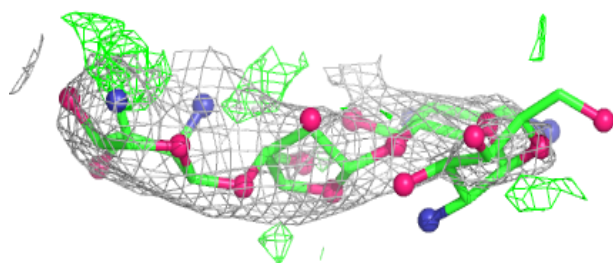
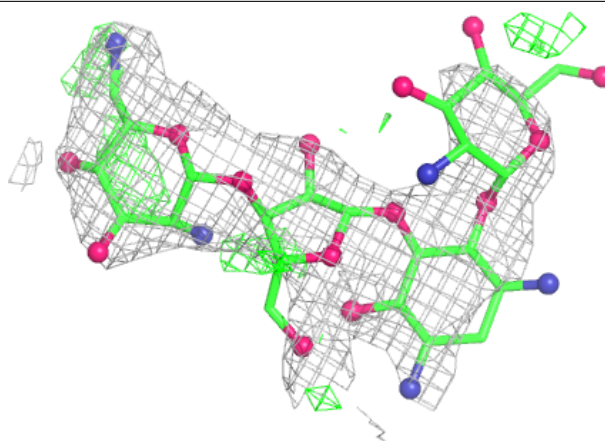
**Electron density around PAR A 1607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



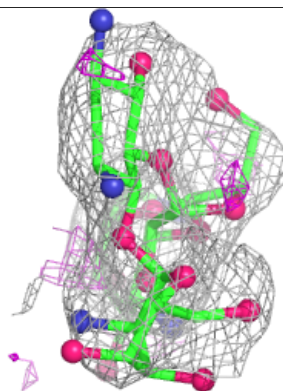
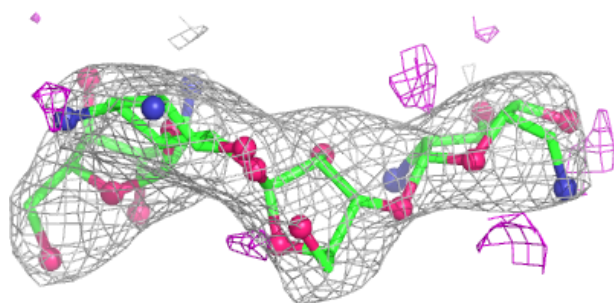
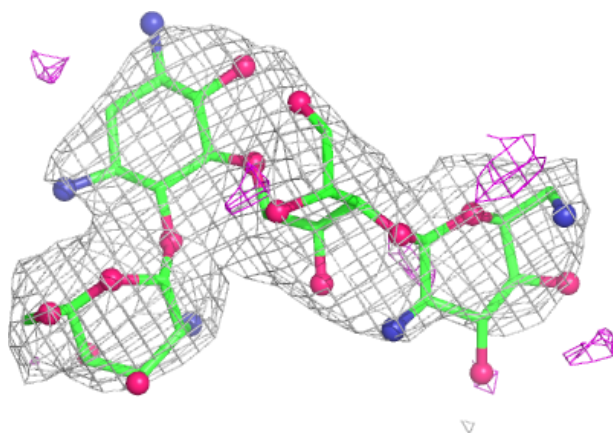
**Electron density around PAR A 1606:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

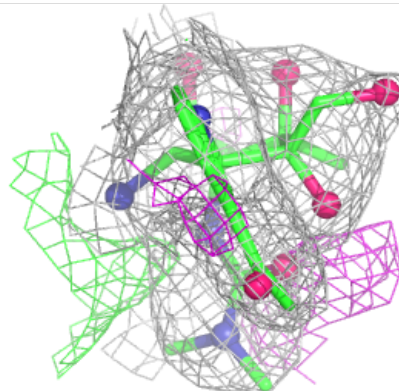
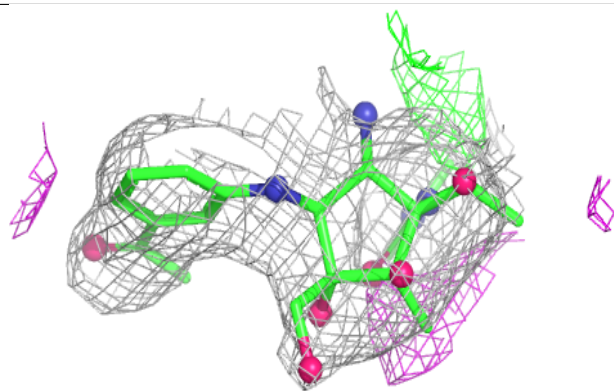
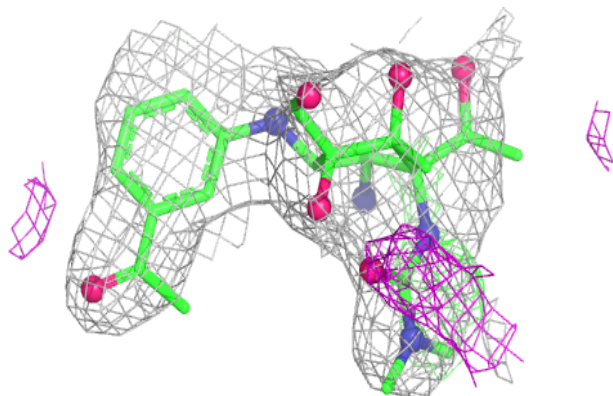


**Electron density around PAR A 1604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

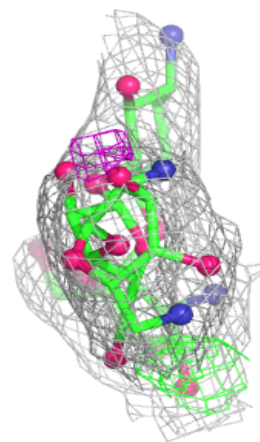
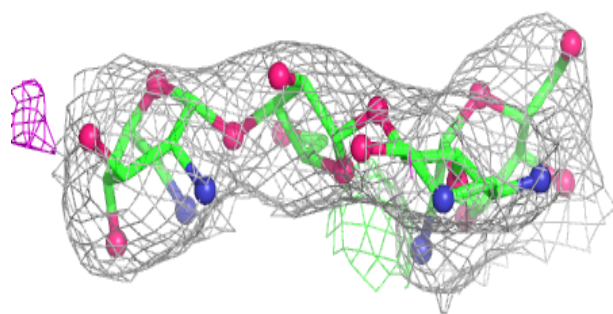
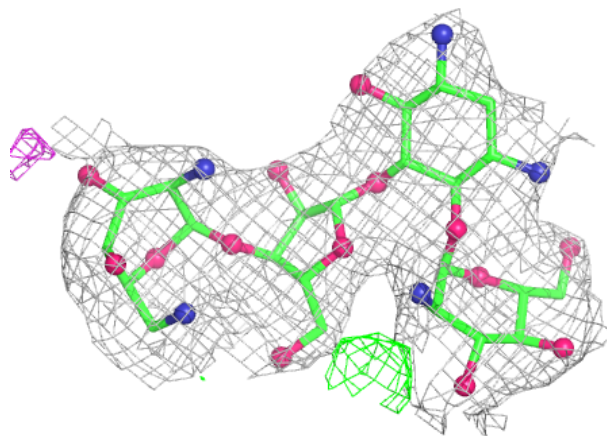
**Electron density around PCY A 1608:**

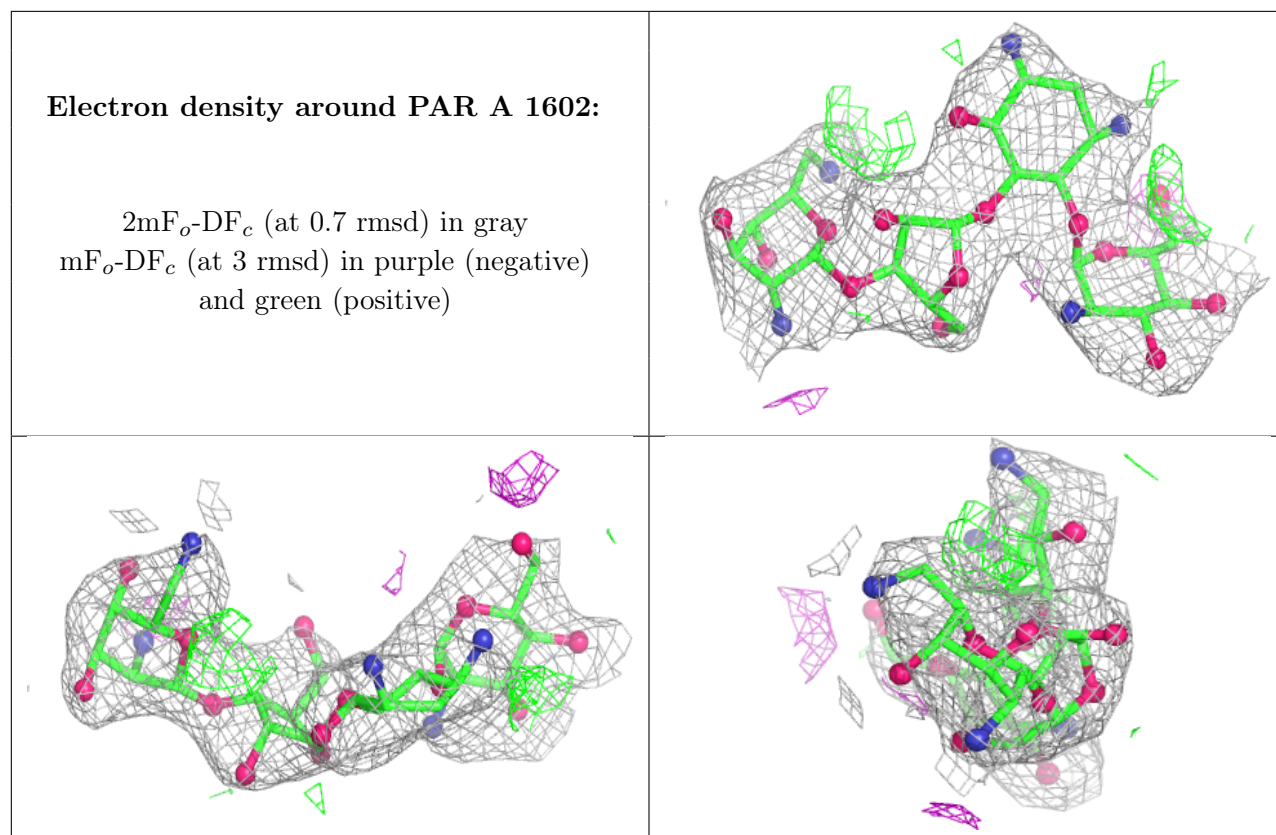
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR A 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.